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Article

Modeling and simulation of liquid metal battery (LMB) materials development using statistical package for social sciences (S.P.S.S.)

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Abstract: There are a number of input parameters that are considered in relation to the stimulatory possibility of constructing a Liquid Metal Battery (LMB). This paper talks about the modeling approach possible for use in LMB research work. Equivalent Circuit Modeling (ECM) is the most common method used to analyze input data or parameters. In analyzing some of the basic elements, such as electrical capacitance, electrical resistance, open circuit voltage, terminal voltage, temperature, time response, time constants, State of Charge (SOC), etc., the cell impedance could be calculated by predicting the system elements that would play key roles in the determination of the parameter identification method for the battery's Equivalent Circuit Model. Secondly, each element in the model has a known behaviour, which mainly depends on the element type and the values of the parameters that characterize that element. In EIS software, the Graphical Model Editor could be used to build an equivalent circuit model, or the befitting model could be carefully and properly selected. Thirdly, in fitting the Equivalent Circuit Model (ECM) to the initial data or parameters, one must take note that the parameters are strongly dependent on temperature, heat, and losses. Such are: the Open Circuit Voltage (OCV), which is strongly dependent on the temperature, the loss processes depend on temperature; losses produced by the loss processes are dissipated as heat energy; the heat generated or consumed by the electrochemical reactions during normal operation has a defined temperature; and a system with a defined temperature window with safe, stable, and efficient operation is achievable. At the end of this research, the simulation of Lithium (Li) and Cadmium (Cd) was found to be in the proportion of 67:33, which is used to determine the strength of the reactivity of the metals. It can be informed in this article that the Bi and Li chemical compositions of the metals are equal to 49 for Li and 51 for Bismuth, which makes the overall reactivity very high, which could be used for LMB development.

Keywords: LMB; energy; Lithium; Cadmium; Antimony; Bismuth; estimation; storage; development

1. Introduction

Despite the known problems of power unavailability due to power outages or insufficiencies, the development of alternative solutions is necessary. The alternative solution needed for electrical energy storage is the LMB [1]. This is mainly done in three ways: the design of batteries with a greater energy density; and the reduction and optimization of dynamic modes of charging/discharging of the LMB. Liquid Metal Batteries (LMBs) compared to other battery types have a number of advantages, which are: greater efficiency, increased energy density, increased nominal voltages, increased lifetime, faster and more efficient charging, no need for routine maintenance, and greater resistance to external conditions [2]. One of the peculiar advantages of LMB is that it does not completely discharge like other conventional batteries. In the field of battery modeling, many different battery models have been proposed in the literature. The battery models can be divided into analytical, electrochemical, and electrical circuit models or a combination of the model types. Analytical models do not give a good outlook on the electrochemical processes occurring in the cell. Electrochemical models require a large amount of computational power to solve the time-varying partial differential equations and cannot be directly linked to the rest of the system [3]. Combined analytical and electrochemical models also suffer from high complexity and poor system modeling compatibility. On the other hand, electrical circuit models can easily be connected to the rest of the electronic systems. However, to model the general behavior of the battery, electrical circuit models are sufficient [4]. Most electrical circuit models can be classified as impedance or thevenin models. Impedance models require Equivalent Circuit Modeling (ECM) to determine the circuit components that are related to the electrochemical processes in the cell [5]. The goal of this paper is to provide a tool for simulating the behaviour of LMB parameters such as the electropositive metal, the electronegative metal, and the suitable molten salt electrolyte under possible simulating conditions, especially with simulation programs such as Matlab software.

2. Battery modelling consideration

Because of the complex charging/discharging characteristics and relative damageability of batteries generally, it is necessary to establish accurate battery models, which can help the design of charging stations more proficiently and dependably. Researchers around the world have developed a wide variety of battery models with varying degrees of impedance. The two primary modeling strategies are the mathematical and circuit-oriented modeling strategies. Conventionally, mathematical battery models are developed based on primary forecast system-level behaviour such as battery runtime, efficiency, or capacity levels [6].

Many recent mathematical battery models have been significantly improved by adding and modifying the terms of conventional battery models to relax the assumptions of the model. This is considered to be able to represent the battery voltage dynamics more accurately when the current varies, as well as when considering battery age and charge/discharge dynamics. Circuit-oriented battery models are electrical equivalent models using a combination of voltage sources, resistors, etc., which are normally used by electrical engineers for designing and co-simulating with other electrical circuits and systems. In modeling generally, a substantial clarification can be made between the electric circuit components of the model and the actual battery dynamics consideration. An equivalent circuit model needs to be built primarily to match experimental data. Such a model provides adequately correct information that serves the need for a real-time battery management approach when properly designed [6].

3. Criteria for battery modelling

To achieve the objectives of the study, the following criteria need to be set according to the different model characteristics, which are presented as follows:

Criteria 1: The model should be able to determine the development of input battery parameters, including terminal voltage, open circuit voltage, the state of health, resistance, etc., which explain the state of the battery for a dynamic discharging condition. It should also be able to adequately represent dynamic processes while the battery is discharging [7].

Criteria 2: The complication of the model should adequately suit Criteria 1 but must also be executable in real-time for a model-based system [7].

Criteria 3: The output of the battery model should be comprehensible to battery operators and technicians, as well as significant to those who do not have any background in battery technologies [7].

4. Different battery model criteria

Many electrochemical factors contained in the electrochemical model are immaterial to the external circuit, and some of the key parameters, like the internal resistance, are hard to explain in an electrochemical model. Therefore, this model technology is not able to meet Criteria 1. However, the solutions in the electrochemical model are not complicated. Criteria 2 can therefore be satisfied by an electrochemical model of a battery. Criteria 3 might be difficult to obtain for an electrochemical model because the understanding of the outputs for an electrochemical model usually requires some background knowledge of the battery chemistry. As a result, the electrochemical model was not chosen for this research work. Physical models can give a good understanding of the battery's important parameters so that Criteria 1 can be satisfied. Criteria 3 can also be met, as the terminal voltage can be determined as the output with the knowledge of these parameters. One significant disadvantage is that the physical models involve a huge amount of calculation in analysis which is quite time-consuming. In finite element or Computational Fluid Dynamics (CFD) methods, a large non-linear system of equations is solved iteratively, and it could take much Central Processing Unit (CPU) time, especially when the system has more than two dimensions. However, the physical modeling methods could also meet Criteria 2, though a fast response is required.

Therefore, Criteria 1 can be satisfied by the equivalent circuit model. The model's ease is due to its low computational time (Criteria 2) and therefore it can be suitable for online implementation [7]. Furthermore, the basic battery parameters like internal resistance, terminal voltage, State of Charge (SOC), etc. can be chosen as the main output of the model to meet Criteria 3.

5. Battery modelling techniques

A number of diverse types of battery models include Electrochemical Model (EM), Computational Fluid Dynamics Model (CFD), Finite Element Model (FEM) and Equivalent Circuit Model (ECM). This part gives a summary of the above-named four various types of battery models and the problems that are solved by each of them. In this part, every battery model technology is judged based on the general criteria.

5.1. Electrochemical model (EM)

The electrochemical model (EM) deals with electrochemistry, which is a division of chemistry that involves chemical reactions that take place in a solution at the interface of an electron conductor (a metal or a semiconductor) and an ionic conductor (the electrolyte). The reactions involve electron transfer between the electrode and the electrolyte. The behaviour of the battery is dependent not only on how it is used but also on a number of construction factors, which are the thickness of the plates, the active mass density of the active material, the concentration of the overall solution, and the nature of the electrodes [8].

5.2. Physical model (PM)

(a) The finite element method (FEM) is that part of the physical model, which deals with numerical analysis techniques for finding estimated solutions to partial differential equations as well as integral equations. The basic principle of the Finite Element Model (FEM) is to divide the problem into elements (parts or portions), and each element or part is a smaller problem to be solved so that they can be analyzed separately. The 'elements' are then assembled together to restore the initial problem. Finite element analysis is a very popular method of analysis in areas with complex geometries like the Liquid Metal Battery (LMB), and it is excellent at stress and thermal analysis of the LMB. The Finite Element Model (FEM) application for batteries could help, especially with a good knowledge of heat loss. There are also attempts to analyze the current density on the positive terminal of the LMB using the FEM analysis tool [8].

(b) Computational Fluid Dynamics (CFD) technology is a well-established tool for the physical analysis and optimization of fluid flow, mass and heat transfer, and related phenomena (e.g., chemical reactions) that may simultaneously take place in a complex system. Therefore, such modeling is able to give an excellent understanding of the battery parameters and detailed characteristics of battery dynamics [8].

5.3. Equivalent circuit model

An equivalent circuit refers to the simplest form of a circuit that retains all of the electrical characteristics of the original circuit. In its most common form, an equivalent circuit is made up of linear, passive elements. However, more complex equivalent circuits are used to approximate the non-linear behaviours of the original circuit. The extensively used equivalent circuit model consists of the battery's Open Circuit Voltage (OCV), ohmic resistance (R0) of the connectors, electrodes, electrolyte, and two parts of parallel resistor-capacitor combinations R1, C1, and R2, C2, representing both the mass transport and the double layer characteristics [8].

$$Vt = V0C - V0 - V1 - V2 \quad (1)$$

$$V0 = iR0 \quad (2)$$

$$C1\frac{dv1}{dt} + \frac{V1}{R1} = I \quad (3)$$

$$C2\frac{dv2}{dt} + \frac{V2}{R2} = I \quad (4)$$

From the Equivalent Circuit Model stated in **Figure 1** above, it was assumed that the battery was de-energized by opening the circuit. A step change in the magnitude of current, occurs for the current, I at t = T0 = 0. The corresponding battery voltage would immediately drop at time, T0 due to the ohmic resistance. Hence, when the circuit is energized due to the closure of the circuit, the current pulse ends at t = T1, which means that the battery voltage has an automatic increment, which is again due to the ohmic resistance factor. Finally, it moves into the time-off stage, where the battery is not charging or discharging. The voltage levels differ exponentially at the time-off stage. Assume that the data is recorded until t = T2.

$$Voc = Vt\ (T0–) \quad (5)$$

To ascertain battery models of superior worth, model parameters need to be correctly calculated from experimental data. To recognize the parameters, usually specific tests such as constant current pulse discharge and charge tests at various SOC and current levels are performed. The ohmic resistance R0 can be easily considered based on the instant battery voltage change before and after the current step. However, the other parameters (R1, C1, and R2, C2) are more difficult to identify because two-time constants are involved in the model.

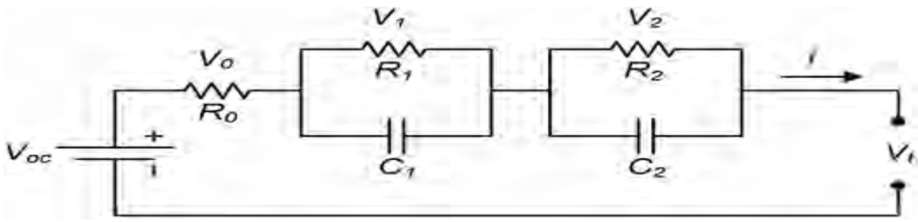

Figure 1. Battery equivalent circuit model [9].

6. Modelling of the battery cell voltage (CV)

The modeling of the battery cell is voltage-based, and it is a function of Discharge Capacity (DC), Charge time (Ct), and Charge Capacity (CC).

$$CV = f\ (DC, Ct, CC) \quad (6)$$

$$CV = α0 + α1DC + α2Ct + α3CC \quad (7)$$

$$CVe = α0e + α1DCe + α2Cte + α3CCe \quad (8)$$

where, CV = Cell Voltage, DC = Discharge Capacity, Ct = Charge time, CC = Charge Capacity, and α signifies a specified constant, which ranges from 0, 1, 2, 3 … ∞.

Equations (6–8) are the model for the battery and the model operates with the parameters CV, DC, Ct, and CC.

$$\text{Temperature (T)} = f\ (\text{time}) \quad (9)$$

$$\text{Open Circuit Voltage (OCV)} = f\ (\text{State of Charge}) \text{ or } f\ (SOC) \quad (10)$$

$$\text{Resistance (R)} = f\ (SOC) \quad (11)$$

$$\text{Capacitance (CP)} = f\ (SOC) \quad (12)$$

$$\text{Time constant (TC)} = f\ (SOC) \quad (13)$$

Hence,

$$SOC = f\ (OCV, R, CP, TC) \quad (14)$$

$$\frac{dE}{dt} = \left(\frac{dE}{dt}\right)\text{gen.} + \left(\frac{dE}{dt}\right)\text{loss} + \left(\frac{dE}{dt}\right)\text{in} + \left(\frac{dE}{dt}\right)\text{out} \quad (15)$$

Table 1 shows the estimated parameters of the Liquid Metal Battery (LMB) with four (4) samples of Liquid Metal Battery developmental parameters, which gives a breakdown into electrode composition, operating temperature, electrode area, inter-electrode distance, charge-discharge current, coulombic efficiency, voltage efficiency, average discharge voltage, theoretical capacity, discharge capacity, voltage input, and voltage output.

Table 1. Estimated parameters for the LMB.

Design parameters	Li//Cd-Sb	Li//Cd-Bi	Li-Bi	Li-Cd
Electrode composition in moles	47-36-17 48-36-16 49-35-16 50-34-16	42-38-20 47-33-20 45-35-20 44-32-24	45-55 40-60 50-50 48-52	70-30 60-40 50-50 65-35
Operating temperature in O °C	450–500	400–500	350–400	300–400
Electrode area in cm^2	1.30–2.50	1.00–1.50	1.00–2.00	1.50–2.00
Inter-electrode distance in cm	1.00–1.50	1.00–2.00	1.50–2.00	1.50–2.00
Charge–discharge current, A	0.34–0.55	0.34–0.55	0.34–0.55	0.34–0.55
Coulombic efficiency in %	80–99	80–99	80–99	80–99
Voltage efficiency in %	65–80	65–80	65–80	65–80
Average discharge voltage in Volts	0.65–0.75	0.65–0.75	0.65–0.75	0.65–0.75
Theoretical capacity in Ah	0.75–0.90	0.75–0.90	0.75–0.90	0.75–0.90
Discharge capacity in Ah	0.55–0.80	0.55–0.80	0.55–0.80	0.55–0.80
Voltage input in Volts	12.0 12.1 12.3 11.9	12.5 12.6 11.8 12.0	11.6 11.7 11.9 12.1	11.5 11.6 11.8 11.7
Voltage output in Volts	220 215 225 235	225 220 230 230	230 225 235 225	235 230 240 220

7. Simulation and analysis of the liquid metal electrodes

From **Figure 2**, a comparison of the reactivity dynamics between the two metals, Bismuth (Bi) and Lithium (Li) shows a variation in the extent of reactivity of the metals involved. From the graph, Lithium is more reactive than Bismuth, which therefore implies that the selection of Lithium metal is suitable. However, the reactivity level of Bismuth was characterized by a slow reaction at the beginning and a spontaneous reaction occurring at the end, though the electrode compositions of Li and Bi are not the same.

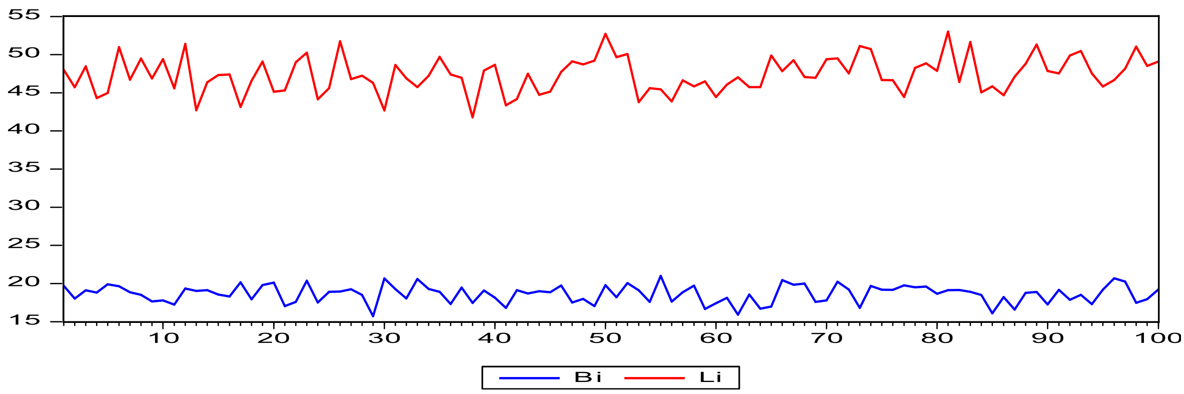

Figure 2. Simulated graph of Bismuth and Lithium metals.

In **Figure 3**, a comparison of the reactivity dynamics between the two metals, Bismuth and Antimony, was done in order to establish the compatibility of both metals. From the graph, Antimony is more reactive than Bismuth, which gives rise to the selection of Antimony metal over Bismuth in terms of the suitability of both metals involved. However, the reactivity level of Antimony was characterized by a fast reaction occurring during the reaction process.

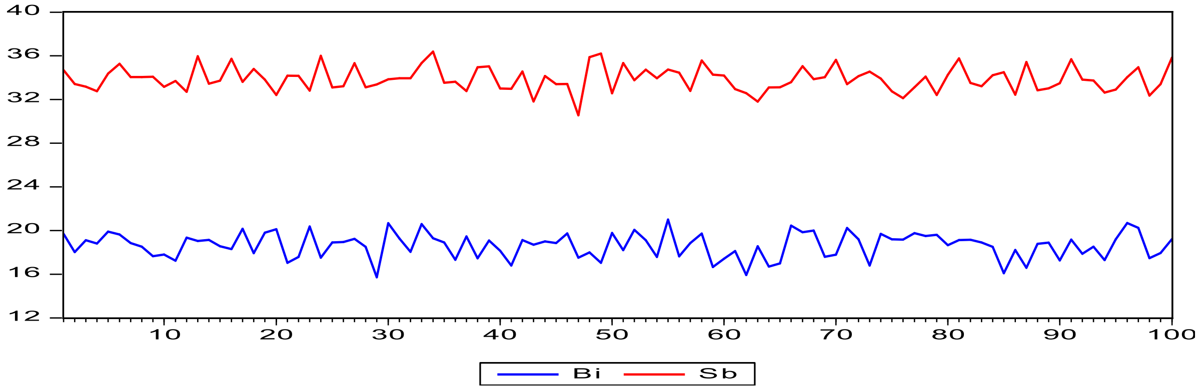

Figure 3. Simulated graph of Bismuth and Antimony metals.

In **Figure 4**, the reactivity dynamics of three metals are x-rayed. The metals are Lithium, Antimony, and Bismuth. The strength of the reactions of the different metals is displayed in the graph above. Lithium indicated in red is highly reactive due to its usual property of being extreme in terms of reactivity. Lithium is followed by Antimony, which is moderately reactive in its alloy combinations in order to decrease the temperature of its overall reactants to give the desired products.

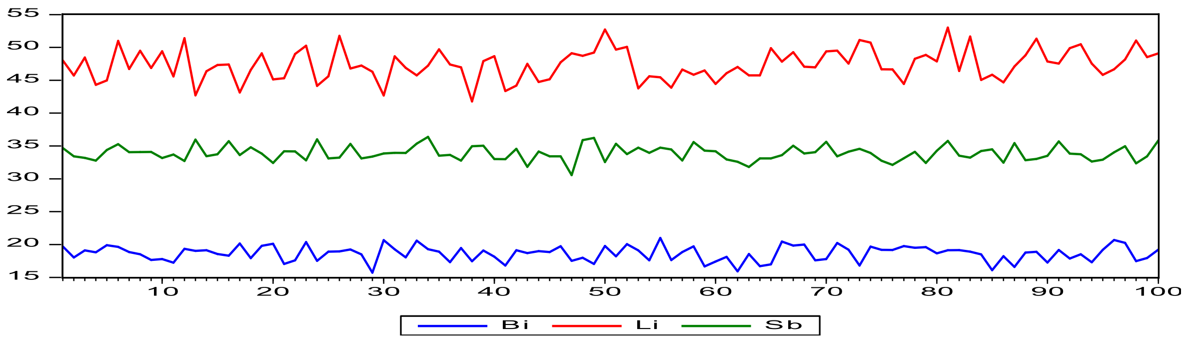

Figure 4. Simulated graph of Bismuth, Lithium, and Antimony metals.

In **Figure 5**, the reactivity of the two metals was examined. The Lithium and Bismuth metals are displayed in the graph above. The Lithium indicated with a red line was moderately reactive. Lithium is followed by Antimony, which is moderately reactive in its alloy combinations, and it helps to decrease the temperature of its overall reactants to give the desired products.

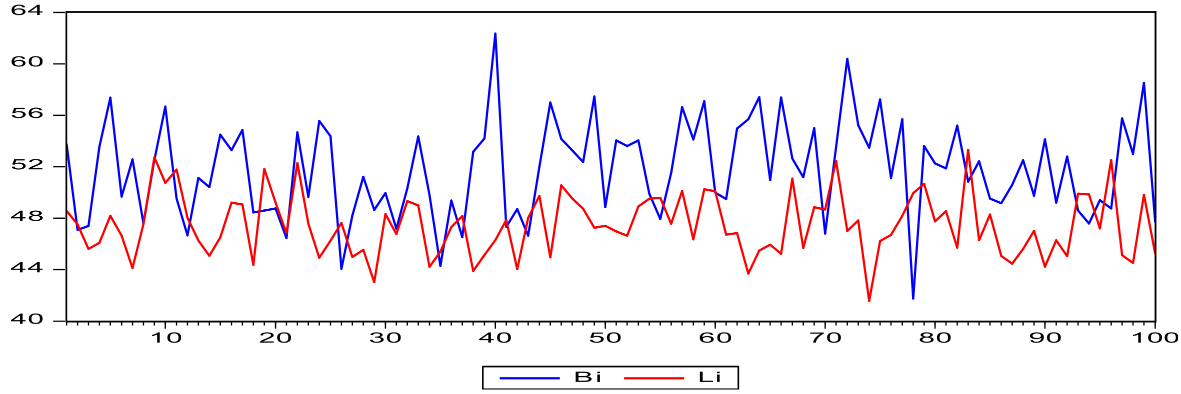

Figure 5. Simulated graph of Bismuth and Lithium metals.

In **Figure 6**, the composition of Lithium (Li) and Cadmium (Cd) was on the premise of 67:33 in order to determine the strength of the reactivity of the metals. From the Bi and Li metals, the chemical composition is almost equal at a ratio of 49 for Li and 51 for Bismuth. The overall reactivity is going to be very high. Thus, the values of the composition are not fit for use in the LMB construction.

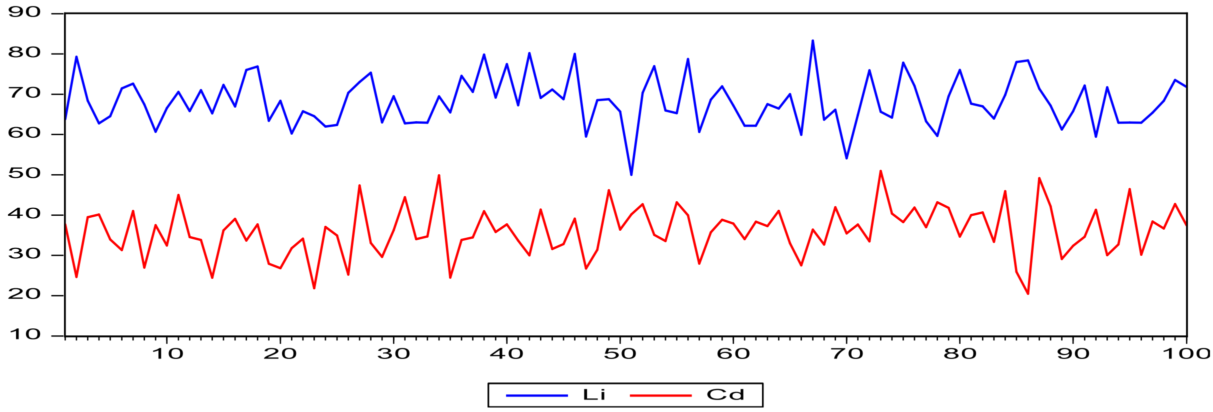

Figure 6. Simulated graph of Lithium and Cadmium metals.

8. Conclusion

From the simulated graphical analysis in this research work, it was deduced that the dynamic characteristics of the LMB metals, which were carefully analyzed, show that the metals Li//Sb-Bi are the most suitable electrodes that could be used among the varieties of proposed metals being examined. The possibility of examining varying salt electrolytes was carried out, and it was discovered that the LiCl-LiF-LiI salt electrolyte is one of the best alternative chemistries. In this paper, the electropositive metal, the electronegative metal, and the molten salt electrolyte were carefully identified and simulated. Based on the simulated results, LMB development is achievable.

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